Towards the Next Generation Air Quality Modeling System: Current Progress on Implementing Chemistry into MPAS-A

Hosein Foroutan, David C. Wong, Jonathan E. Pleim, O. Russell Bullock Jr., Robert C. Gilliam, Jerold A. Herwehe, George A. Pouliot, Christian Hogrefe

Computational Exposure Division, National Exposure Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, RTP, NC, USA

contact email: foroutan.hosein@epa.gov

Introduction

Air quality issues need to be addressed globally recognizing the linkages and interactions between meteorology and atmospheric chemistry across a wide range of scales. Therefore, an effort is currently underway at the United States Environmental Protection Agency (US EPA) to develop a next-generation air quality modeling system (NGAQM) that will be based on a global integrated meteorology and chemistry system.

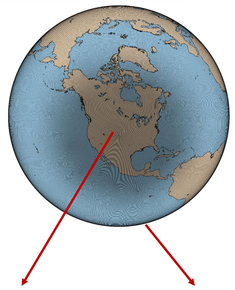
The Model for Prediction Across Scales-Atmosphere (MPAS-A) developed by the National Center for Atmospheric Research (NCAR), a global fully compressible non-hydrostatic model with seamlessly refined centroidal Voronoi grids, has been chosen as the meteorological driver of this modeling system.

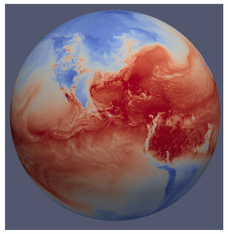
The initial step of adapting MPAS-A for the NGAQM was to implement and test the physics parameterizations and options that are preferred for retrospective air quality simulations. The next step, presented herein, would be to link the chemistry from the Community Multiscale Air Quality (CMAQ) model of the US EPA to MPAS-A to build a prototype (MPAS-AQ) for the NGAQM.

MPAS-AQ Configurations

MPAS-A configurations

- MPAS-A v4.0
- 92-25 km mesh (refined over the CONUS)
- 50 vertical grids expanding up to 30 km (first grid at ~18 m)
- RRTMG SW and LW radiation and WSM6 microphysics
- Pleim-Xiu land-surface model (PX LSM), Asymmetric Convective Model 2 PBL model (ACM2), Pleim surface layer model (PSL), and Kain-Fritsch (KF) convective parametrization as in WRF v3.8 (implemented by the US EPA)
- Four Dimensional Data Assimilation (FDDA) (implenented by the US EPA)

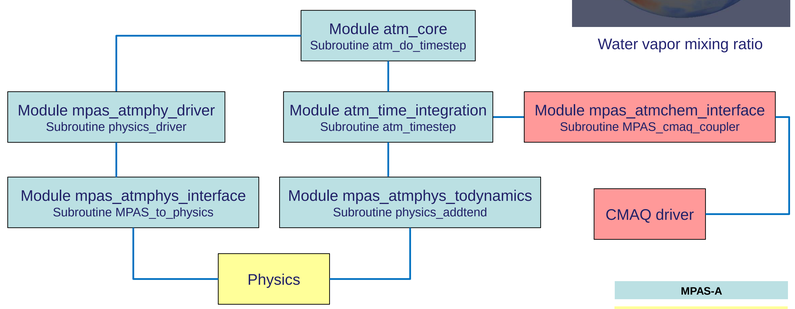




Water vapor mixing ratio

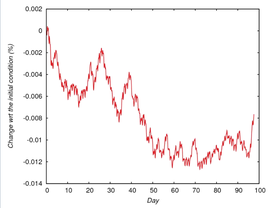
Chemistry Configurations

- Gas-phase chemistry only
- Carbon Bond mechanism as in CMAQ v5.1 (CB05e51)
- Euler backwards iterative solver (EBI)

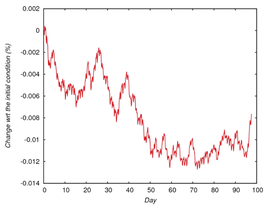


Schematic diagram of the MPAS-AQ prototype

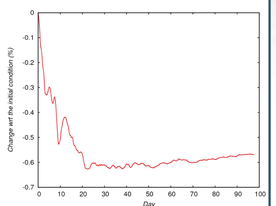
Mass Conservation Experiments



Changes in the total mass of the dry air ($\int_D \rho \, dV$) in the domain



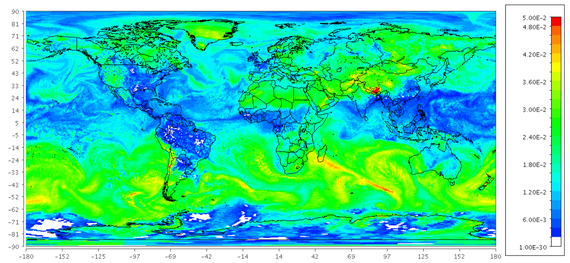
Changes in the total mass of tracer1 ($\int_D \rho \, q_1 \, dV$) in the domain (I.C. = uniform)



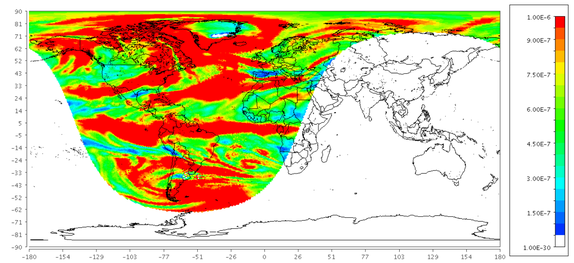
Changes in the total mass of tracer2 ($\int_D \rho \, q_2 \, dV$) in the domain (I.C. = 0.02 × q_v)

MPAS-AQ Preliminary Simulations

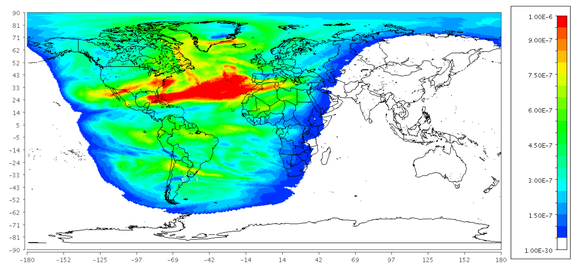
- June 1-7, 2016 simulation period
- Smooth vertical profile (20 ppmv – 8000 ppmv) for O_3 initial condition
- Clean initial condition (1×10^{-20} ppmv) for all other species



O_3 concentrations (ppmv) at layer 1 (~18 m) on 17:00 UTC June 7 2016

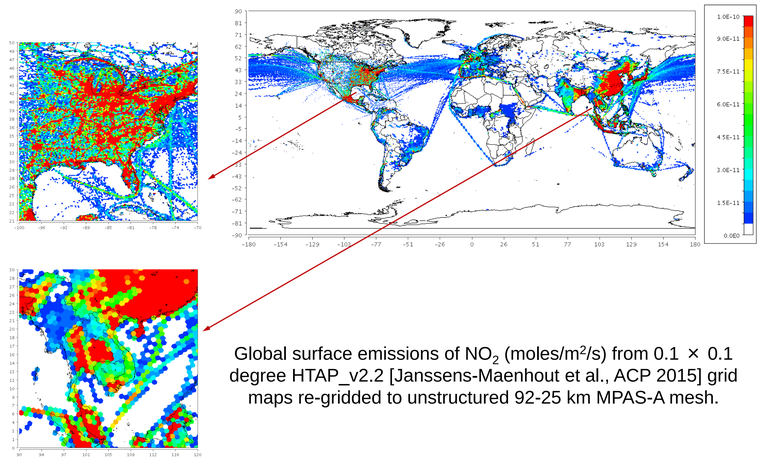


O concentrations (ppmv) at layer 45 (~21 km) on 17:00 UTC June 7 2016



OH concentrations (ppmv) at layer 45 (~21 km) on 17:00 UTC June 7 2016

Global Emissions for MPAS-AQ



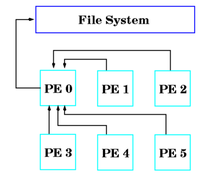
Global surface emissions of NO_2 (moles/m^2/s) from 0.1 × 0.1 degree HTAP_v2.2 [Janssens-Maenhout et al., ACP 2015] grid maps re-gridded to unstructured 92-25 km MPAS-A mesh.

Coupler and I/O Structure

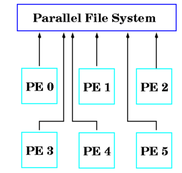
For this MPAS-AQ prototype, we instrumented a coupler that bridges MPAS-A and the Chemistry module (CHEM) with three functions:

- Transfer required meteorological data and concentration data from MAPS-A to CHEM with rearranging data dimension order
- Convert certain meteorological data into a suitable format for CHEM
- Transform concentration information from CHEM back to MPAS-A

On the I/O, we have designed a library that handles various netCDF data formats: WRF, MPAS-A, and IOAPI_3. Our long term goal is to provide flexible capabilities to couple air quality model with global models such as MPAS-A and regional models such as WRF, and to execute it in a stand alone mode. This I/O library allows input and output function operates in serial, pseudo-parallel, and true-parallel mode (see figures below).



Pseudo-parallel



True-parallel

Ongoing Research

- Expand the chemistry module to include aerosols.
- Further develop the I/O system and read in emissions data.
- Conduct long-term and detailed evaluations against observations.
- Develop model science and algorithms expandable to global scale, e.g.,
  - Continue advances in organic aerosols and new particle formation.
  - Develop integrated cloud model with convective transport, microphysics, aqueous chemistry, and aerosol-cloud interactions.
  - Develop emission process modeling for global coverage – (dust, biogenic, bidirectional flux, fires).